SUNDIALS

SUite of Nonlinear and DIfferential/ALgebraic equation Solvers

Overview

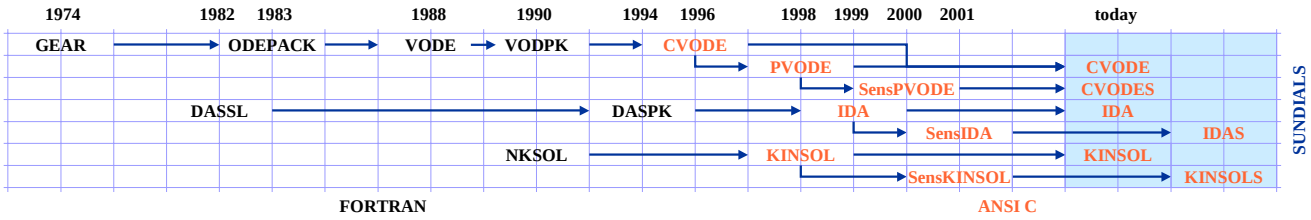
A flexible suite of solvers for time integration and solution of large-scale nonlinear systems of ordinary differential, differential/algebraic, and partial differential equations, including optional solves for sensitivities with respect to model parameters

- Adaptive time integrators and solvers
  - ODEs, y'=f(t, y, p), `CVODE`
  - DAEs, F(t, y', y, p) = 0, `IDA`
  - Algebraic systems, F(y, p) = 0, `KINSOL`
- Builds on LLNL history of general purpose software packages
  - Among the most widely used solvers for these problems (ODEPACK, VODE)
- Data structure neutral approach
  - Allows users to supply their own data structures for kernel operations
- Time integration is variable order, variable step size
  - BDF up to order 5 (for stiff systems & DAEs)
  - Adams (for nonstiff ODEs)
- Nonlinear systems solved by inexact Newton method
- Linear solvers provided
  - GMRES
  - Direct (dense and banded)
  - Interfaces for user-supplied linear solvers and preconditioners

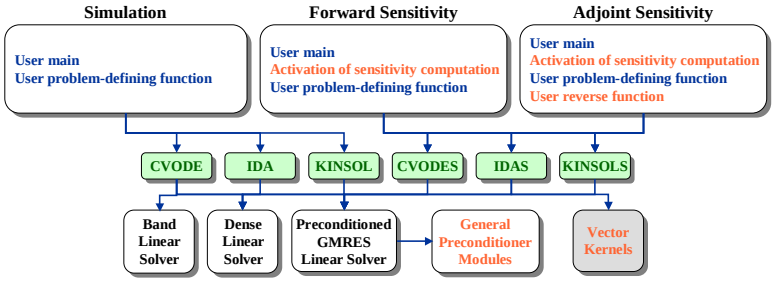
Sensitivity Analysis

Quantitative measure of how the variation in the output of a model can be apportioned to different sources of variation in the input. Sensitivity results can be used in model evaluation, model reduction, data assimilation, uncertainty quantification, and optimization

- Forward sensitivity approach
  - Most effective for computing sensitivities with respect to a few parameters
  - Based on integrating so-called sensitivity equations in tandem with the original system
- Implementation approaches
  - Simultaneous corrector
  - Staggered corrector
- Adjoint sensitivity approach
  - Most effective when computing gradients of a few derived functionals with respect to any number of parameters
  - Based on integrating the adjoint system backwards in time
- Implementation
  - Check-pointing
  - Cubic Hermite interpolation



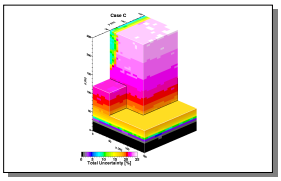
Package Structure



User Interface

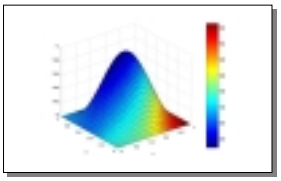
- Users can supply their own data structures underneath SUNDIALS
- Implementation of vector module must include
  - Content of a vector environment
  - Implementations of vector operations (dot products, norms, scalings)
  - Routines to construct the environment and attach the list of operations
- SUNDIALS provides default serial and parallel vector implementations
- Users supply the problem-defining function, F or f.
- Users can supply their own preconditioner set-up and solve routines

Applications



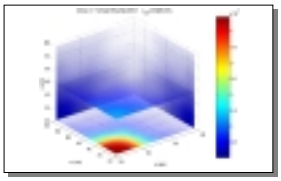
Uncertainty quantification for groundwater simulation

Variably saturated flow model
Study relative importance of parameters in relative permeability
First order uncertainty, based on sensitivities computed with the forward approach, is color-coded
SensKINSOL



Sensitivity analysis in a population dynamics model

Six-species predator-prey model with reaction and diffusion
Study influence of ICs on average population
Height represents IC for species 1
Sensitivities, computed with the adjoint approach, are color-coded
CVODES



Sensitivity analysis in neutral particle transport simulation

Time-dependent, 3-energy group Boltzmann transport model
Study influence of cross section parameters on solution
Solution is color-coded
Sensitivity is coded through transparency
SensIDA

The SUNDIALS Team

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Publications

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